On the properties of the solution path of the constrained and penalized L2-L0 problems

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1 Domain of optimization

For $k \leqslant n$, we define the domain $\mathcal{D}_k \subset \mathbb{R}^n$:

$$\mathcal{D}_k \quad = \quad \{\boldsymbol{x} \in \mathbb{R}^n,\ \|\boldsymbol{x}\|_0 = k\}. \tag{1}$$

Theorem 1 *For $k \geqslant 1$, $\mathcal{D}_k$ is not a closed set, and $\overline{\mathcal{D}_k} = \{\boldsymbol{x} \in \mathbb{R}^n,\ \|\boldsymbol{x}\|_0 \leqslant k\}$ (denoting by $\bar{\ }$ the closure operator).*

Proof 1

- *$\mathcal{D}_k$ is not a closed set: it is easy to find a sequence $\boldsymbol{x}_j \in \mathcal{D}_k$ $(j \in \mathbb{N})$ whose limit is not in $\mathcal{D}_k$. For instance, $\boldsymbol{x}_j = (1/j)\,\boldsymbol{e}$, where $\boldsymbol{e}$ is a given vector in $\mathcal{D}_k$. $\boldsymbol{x}_j$ tends towards $\mathbf{0} \notin \mathcal{D}_k$.*
- *$\overline{\mathcal{D}_k} \subseteq \{\boldsymbol{x} \in \mathbb{R}^n,\ \|\boldsymbol{x}\|_0 \leqslant k\}$. If $\boldsymbol{x} \in \overline{\mathcal{D}_k}$, then there exists a sequence $\boldsymbol{x}_j \in \mathcal{D}_k$ $(j \in \mathbb{N})$ whose limit is equal to $\boldsymbol{x}$. Then,*
  $$\forall \varepsilon > 0,\ \exists J,\ j \geqslant J \Rightarrow \forall i,\ |\boldsymbol{x}(i) - \boldsymbol{x}_j(i)| < \varepsilon.$$
  Applying this property with $\varepsilon = \min\limits_{\boldsymbol{x}(i) \neq 0} |\boldsymbol{x}(i)|$, we deduce that there exists an iteration J, such that $\forall j \geqslant J$, $\forall i$, $\boldsymbol{x}(i) \neq 0 \Rightarrow \boldsymbol{x}_j(i) \neq 0$. In other words, $\|\boldsymbol{x}\|_0 \leqslant \|\boldsymbol{x}_j\|_0 = k$.
- *$\{\boldsymbol{x} \in \mathbb{R}^n,\ \|\boldsymbol{x}\|_0 \leqslant k\} \subseteq \overline{\mathcal{D}_k}$. Let us show that if $\boldsymbol{x}$ is such that $\|\boldsymbol{x}\|_0 \leqslant k$, then there exists a sequence $\boldsymbol{x}_j \in \mathcal{D}_k$ whose limit is equal to $\boldsymbol{x}$. Given $\boldsymbol{x}$, we define $\boldsymbol{x}_j$ by setting $\boldsymbol{x}_j(i) = \boldsymbol{x}(i)$ if $i \in \mathcal{A}(\boldsymbol{x})$ (support of $\boldsymbol{x}$), and by replacing the $k - \|\boldsymbol{x}\|_0$ first zero valued entries of $\boldsymbol{x}$ by $1/j$ in $\boldsymbol{x}_j$, and setting to 0 the remaining $n-k$ entries $\boldsymbol{x}_j(i)$. Obviously, $\boldsymbol{x}_j \in \mathcal{D}_k$ and this sequence tends towards $\boldsymbol{x}$.*

The consequence of theorem 1 is that

$$\operatorname*{arg\,min}_{\boldsymbol{x} \in \mathcal{D}_k} \{\mathcal{E}(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2\}$$

is not always defined, although the minimal value $\min\limits_{\boldsymbol{x} \in \mathcal{D}_k} \mathcal{E}(\boldsymbol{x})$ is defined. On the contrary, the set of minimizers

$$\mathcal{X}_c(k) = \operatorname*{arg\,min}_{\boldsymbol{x} \in \overline{\mathcal{D}_k}} \mathcal{E}(\boldsymbol{x}) = \operatorname*{arg\,min}_{\|\boldsymbol{x}\|_0 \leqslant k} \mathcal{E}(\boldsymbol{x})$$

is properly defined because $\overline{\mathcal{D}_k}$ is a closed set and $\mathcal{E}$ is quadratic and convex (to be completed).

Example 1 *Let us consider the minimization of $\|\boldsymbol{x}\|^2$ over the domain $\mathcal{D}_k$. For $k \geqslant 1$, there is no minimizer over $\mathcal{D}_k$, but the minimal cost $\min\limits_{\boldsymbol{x} \in \mathcal{D}_k} \|\boldsymbol{x}\|^2$ is equal to 0. The set of minimizers over $\overline{\mathcal{D}_k}$ is reduced to one vector: $\mathcal{X}_c(k) = \{\mathbf{0}\}$.*

Example 2 *The set $\mathcal{X}_c(k)$ is not always a singleton. Let us consider the minimization of the 2D cost function $\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}(1)^2$. It is easy to see that $\mathcal{X}_c(0) = \{\mathbf{0}\}$, $\mathcal{X}_c(1) = \{[0, \boldsymbol{x}(2)]^T,\ \boldsymbol{x}(2) \in \mathbb{R}\}$ and $\mathcal{X}_c(2) = \mathcal{X}_c(1)$.*

Example 3 *Let us consider the minimization of the 2D cost function* $\mathcal{E}(\boldsymbol{x}) = (\boldsymbol{x}(1) - \alpha)^2$ *for a given* $\alpha \neq 0$. *It is easy to see that* $\mathcal{X}_c(0) = \{\mathbf{0}\}$, $\mathcal{X}_c(1) = \{[\alpha, 0]^T\}$ *and* $\mathcal{X}_c(2) = \{[\alpha, \boldsymbol{x}(2)]^T,\ \boldsymbol{x}(2) \in \mathbb{R}\}$.

Remark 1 *Obviously, the sets* $\overline{\mathcal{D}_k}$ *have a nesting property* ($\overline{\mathcal{D}_k} \subset \overline{\mathcal{D}_{k+1}}$)*, therefore, for all* k*, we have*

$$\forall \boldsymbol{x}_k \in \mathcal{X}_c(k), \forall \boldsymbol{x}_{k+1} \in \mathcal{X}_c(k+1),\ \mathcal{E}(\boldsymbol{x}_{k+1}) \leqslant \mathcal{E}(\boldsymbol{x}_k).$$

Theorem 2 $\mathcal{X}_c(k+1) \cap \overline{\mathcal{D}_k} \subseteq \mathcal{X}_c(k)$.

Proof 2 *Let us consider* $\boldsymbol{x}_{k+1} \in \mathcal{X}_c(k+1) \cap \overline{\mathcal{D}_k}$. *Since* $\overline{\mathcal{D}_k} \subset \overline{\mathcal{D}_{k+1}}$ *and* $\boldsymbol{x}_{k+1}$ *is a minimizer of* $\mathcal{E}$ *over* $\overline{\mathcal{D}_{k+1}}$*, we have* $\forall \boldsymbol{x} \in \overline{\mathcal{D}_k}$, $\mathcal{E}(\boldsymbol{x}_{k+1}) \leqslant \mathcal{E}(\boldsymbol{x})$. *As* $\boldsymbol{x}_{k+1} \in \overline{\mathcal{D}_k}$, $\boldsymbol{x}_{k+1}$ *is a minimizer of* $\mathcal{E}$ *over* $\overline{\mathcal{D}_k}$.

2 Working assumptions and notion of constrained solution path

2.1 Unique representation property

We recall the definition of the unique representation property (URP), introduced in [1] in the underdetermined case (when $m \leqslant n$):

Definition 1 *A matrix* $\boldsymbol{A}$ *of size* $m \times n$ ($m \leqslant n$) *satisfies the URP if and only if any selection of* m *columns of* $\boldsymbol{A}$ *forms a family of linearly independent vectors.*

Under the URP assumption, we can solve $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ by imposing that $\boldsymbol{x} \in \overline{\mathcal{D}_m}$. The system is then equivalent to $\boldsymbol{y} = \boldsymbol{B}\boldsymbol{z}$ where $\boldsymbol{B}$ is a matrix of size $m \times m$ extracted from $\boldsymbol{A}$, and $\boldsymbol{z}$ is the corresponding vector extracted from $\boldsymbol{x}$, of size $m \times 1$. According to the URP definition, $\boldsymbol{B}$ is always invertible, and we can find sparse solutions to $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ with at most m non-zero entries ($\boldsymbol{z} = \boldsymbol{B}^{-1}\boldsymbol{y}$ and then $\boldsymbol{x} = \{\boldsymbol{z}, \mathbf{0}\}$ for all the possible extractions $\boldsymbol{B}$ from $\boldsymbol{A}$).

When $m > n$, we adopt the following definition:

Definition 2 *A matrix* $\boldsymbol{A}$ *of size* $m \times n$ ($m > n$) *satisfies the URP if and only if it is full rank.*

When $m > n$, there is generally no solution to $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ but the minimizer of $\mathcal{E}(\boldsymbol{x})$ over $\mathbb{R}^n$ is unique (although not necessarily sparse): $\mathcal{X}_c(n) = \{(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}\}$.

In the following, we will assume that $\boldsymbol{y} \neq \mathbf{0}$ and that $\boldsymbol{A}$ satisfies the URP.

2.2 Cardinality of the set $\mathcal{X}_c(k)$

Theorem 3 *For* $k \leqslant \min(m, n)$*, the set* $\mathcal{X}_c(k)$ *is finite under the URP assumption.*

Proof 3 *Because of the URP assumption, any selection of* $k \leqslant \min(m, n)$ *columns of* $\boldsymbol{A}$ *yields a matrix* $\boldsymbol{B}$ *of size* $m \times k$ *whose rank is equal to* k. *Then, the energy reduces to* $\mathcal{E}(\boldsymbol{x}) = \mathcal{E}(\boldsymbol{z}; \mathbf{0}) = \|\boldsymbol{y} - \boldsymbol{B}\boldsymbol{z}\|^2$ *(where* $\boldsymbol{z} \in \mathbb{R}^k$*), and there is only one minimizer of* $\boldsymbol{z} \mapsto \mathcal{E}(\boldsymbol{z}; \mathbf{0})$ *over* $\mathbb{R}^k$. *Since the number of possible selections of* k *columns of* $\boldsymbol{A}$ *is finite, the set* $\mathcal{X}_c(k)$ *is finite.*

Remark 2 *The minimal value of* $\mathcal{E}(\boldsymbol{x})$ *(for* $\boldsymbol{x} \in \mathbb{R}^n$*) can be reached when minimizing* $\mathcal{E}$ *over* $\overline{\mathcal{D}_{\min(m,n)}}$. *Thus, when* $m \leqslant n$*, it is not necessary to compute* $\mathcal{X}_c(k)$ *for* $k > m$. *According to theorem 3, when* $m > n$*, all the sets* $\mathcal{X}_c(k)$, $k = 0, \ldots, n$ *are finite.*

Theorem 4 *When* $m \leqslant n$ *and* k *is such that* $m < k \leqslant n$*, the set* $\mathcal{X}_c(k)$ *is of infinite cardinality.*

Proof 4 *Given a solution* $\boldsymbol{x}_m \in \mathcal{X}_c(m)$*, let* $\mathcal{A}(\boldsymbol{x}_m)$ *be the support of* $\boldsymbol{x}_m$. *We consider a support* $\mathcal{B}$ *of cardinality* k *such that* $\mathcal{A}(\boldsymbol{x}_m) \subset \mathcal{B} \subseteq \{1, \ldots, n\}$*, and we extract from* $\boldsymbol{A}$ *the matrix* $\boldsymbol{B}$ *of size* $m \times k$ *formed of the columns* $\boldsymbol{a}_i$ *of* $\boldsymbol{A}$ *(*$i \in \mathcal{B}$*). Then, let us add to* $\boldsymbol{x}_m$ *a vector* $\boldsymbol{n}$ *belonging to the null space of* $\boldsymbol{B}$. *Clearly,* $\boldsymbol{x}_m + \boldsymbol{n} \in \mathcal{X}_c(k)$ *because* $\|\boldsymbol{x}_m + \boldsymbol{n}\|_0 \leqslant k$ *and* $\mathcal{E}(\boldsymbol{x}_m + \boldsymbol{n}) = \mathcal{E}(\boldsymbol{x}_m) = \min_{\boldsymbol{x} \in \mathbb{R}^n} \mathcal{E}(\boldsymbol{x})$. *Since the null space of* $\boldsymbol{B}$ *is of dimension* $k - m > 0$, $\mathcal{X}_c(k)$ *is of infinite cardinality.*

As a conclusion, the constrained solution path is defined in the following way, for any case ($m \leqslant n$ or $m > n$).

Definition 3 *The constrained solution path is the (finite) set*

$$\mathcal{X}_c = \bigcup_{k=0}^{\min(m,n)} \mathcal{X}_c(k).$$

3 Properties of the penalized solution path

3.1 Penalized solution path

For a given $\lambda \geqslant 0$, we define the set of minimizers of $\mathcal{J}(\boldsymbol{x};\lambda) = \mathcal{E}(\boldsymbol{x}) + \lambda\|\boldsymbol{x}\|_0$:

$$\mathcal{X}_p(\lambda) = \operatorname*{arg\,min}_{\boldsymbol{x}\in\mathbb{R}^n} \{\mathcal{J}(\boldsymbol{x};\lambda)\}.$$

By extension, we define $\mathcal{X}_p(+\infty) = \{\mathbf{0}\}$.

Definition 4 *We denote the cardinality of a set $\mathcal{A} \subseteq \{1,\ldots,n\}$ by*

$$\|\mathcal{A}\|_0 \triangleq Card(\mathcal{A}).$$

Definition 5 *We denote by $\mathcal{A}(\boldsymbol{x}) \subseteq \{1,\ldots,n\}$ the support of a vector $\boldsymbol{x} \in \mathbb{R}^n$.*

Definition 6 *For a given active set $\mathcal{A}$ such that $\|\mathcal{A}\|_0 \leqslant \min(m,n)$, the corresponding least-square solution is unique (due to the URP assumption). We denote this solution by*

$$\boldsymbol{x}_{\mathcal{A}} \triangleq \operatorname*{arg\,min}_{\mathcal{A}(\boldsymbol{x})\subseteq\mathcal{A}} \mathcal{E}(\boldsymbol{x}) \tag{2}$$

and the corresponding least-square cost by

$$\mathcal{E}_{\mathcal{A}} \triangleq \mathcal{E}(\boldsymbol{x}_{\mathcal{A}}) = \min_{\mathcal{A}(\boldsymbol{x})\subseteq\mathcal{A}} \mathcal{E}(\boldsymbol{x}). \tag{3}$$

Finally, we define the corresponding value of $\mathcal{J}$ by

$$\mathcal{J}_{\mathcal{A}}(\lambda) \triangleq \mathcal{J}(\boldsymbol{x}_{\mathcal{A}};\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda\|\boldsymbol{x}_{\mathcal{A}}\|_0 \tag{4}$$

which is generally different from

$$\min_{\mathcal{A}(\boldsymbol{x})\subseteq\mathcal{A}} \mathcal{J}(\boldsymbol{x};\lambda).$$

Theorem 5 *If $\lambda > 0$ and $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, then the support of $\boldsymbol{x}_p(\lambda)$, denoted by $\mathcal{A} \triangleq \mathcal{A}(\boldsymbol{x}_p(\lambda))$ for convenience, is such that $\|\mathcal{A}\|_0 \leqslant \min(m,n)$, and $\boldsymbol{x}_p(\lambda) = \boldsymbol{x}_{\mathcal{A}}$.*

Proof 5 — *First, we show that*

$$\boldsymbol{x}_p(\lambda) \in \operatorname*{arg\,min}_{\{\boldsymbol{x}\in\mathbb{R}^n,\,\mathcal{A}(\boldsymbol{x})\subseteq\mathcal{A}\}} \mathcal{E}(\boldsymbol{x}).$$

Since $\boldsymbol{x}_p(\lambda)$ is a minimizer of $\mathcal{J}(\boldsymbol{x};\lambda)$, the following equivalent inequalities hold for all $\boldsymbol{x}$ such that $\mathcal{A}(\boldsymbol{x}) \subseteq \mathcal{A}$:

$$\begin{aligned}
\mathcal{J}(\boldsymbol{x};\lambda) &\geqslant \mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda)\\
\mathcal{E}(\boldsymbol{x}) + \lambda\|\boldsymbol{x}\|_0 &\geqslant \mathcal{E}(\boldsymbol{x}_p(\lambda)) + \lambda\|\mathcal{A}\|_0\\
\mathcal{E}(\boldsymbol{x}) - \mathcal{E}(\boldsymbol{x}_p(\lambda)) &\geqslant \lambda\big(\|\mathcal{A}\|_0 - \|\boldsymbol{x}\|_0\big) \geqslant 0.
\end{aligned}$$

We finally deduce that $\boldsymbol{x}_p(\lambda)$ is a minimizer of $\mathcal{E}$ over the set $\{\boldsymbol{x} \in \mathbb{R}^n,\, \mathcal{A}(\boldsymbol{x}) \subseteq \mathcal{A}\}$.
— The case where $\|\mathcal{A}\|_0 > \min(m,n)$ never occurs. If it does, remark 2 shows that there exists $\boldsymbol{x} \in \overline{\mathcal{D}_{\min(m,n)}}$ such that $\mathcal{E}(\boldsymbol{x}) = \mathcal{E}(\boldsymbol{x}_p(\lambda))$. Since $\|\boldsymbol{x}\|_0 \leqslant \min(m,n) < \|\boldsymbol{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0$, $\mathcal{J}(\boldsymbol{x};\lambda) < \mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda)$, which is in contradiction with $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$.

Finally, $\|\mathcal{A}\|_0 \leqslant \min(m,n)$ and there is only one minimizer of $\mathcal{E}$ over the set $\{\boldsymbol{x} \in \mathbb{R}^n,\, \mathcal{A}(\boldsymbol{x}) \subseteq \mathcal{A}\}$ (URP assumption), which is $\boldsymbol{x}_{\mathcal{A}}$.

Corrolary 1 *If $\lambda > 0$, the set $\mathcal{X}_p(\lambda)$ is finite and $\mathcal{X}_p(\lambda) \subseteq \overline{\mathcal{D}_{\min(m,n)}}$.*

Proof 6 *There are at most $\sum_{k=0}^{\min(m,n)} C_n^k$ distinct values $\boldsymbol{x}_p(\lambda)$ (i.e., $\sum_{k=0}^{\min(m,n)} C_n^k$ sets which are candidate to be a set $\mathcal{A}$ and one optimal $\boldsymbol{x}$-value $\boldsymbol{x}_\mathcal{A}$ per set), which shows that $\mathcal{X}_p(\lambda)$ is a finite set. Additionally, we have seen in theorem 5 that for each solution $\boldsymbol{x}_p(\lambda)$, $\|\boldsymbol{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0 \leqslant \min(m,n)$.*

Definition 7 *The penalized solution path is defined as the union of sets*

$$\mathcal{X}_p = \bigcup_{\lambda>0} \mathcal{X}_p(\lambda).$$

Imposing $\lambda > 0$ (rather than $\lambda \geqslant 0$) guarantees that $\mathcal{X}_p(\lambda)$ is of finite cardinality for all λ. Moreover, it is easy to see (from theorem 5) that the solution path is of finite cardinality, since all the sets $\mathcal{X}_p(\lambda)$ are included in a common set of cardinality $\sum_{k=0}^{\min(m,n)} C_n^k$: $\{\boldsymbol{x} \in \mathbb{R}^n,\ \exists \mathcal{A} \subseteq \{1,\ldots,n\},\ \|\mathcal{A}\|_0 \leqslant \min(m,n) \text{ and } \boldsymbol{x} = \boldsymbol{x}_\mathcal{A}\}$.

3.2 Piecewise constant property

Theorem 6 *The dependence of the set $\mathcal{X}_p(\lambda)$ w.r.t. λ ($\lambda > 0$) is piecewise constant, with a finite number of intervals $(\lambda_i^\star, \lambda_{i+1}^\star)$: for all i, $\mathcal{X}_p(\lambda)$ is constant for $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$ and if $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^\star) \cap \mathcal{X}_p(\lambda_{i+1}^\star)$.*

The minimal cost value $\mathcal{J}(\lambda) \triangleq \min_{\boldsymbol{x}\in\mathbb{R}^n} \mathcal{J}(\boldsymbol{x};\lambda)$ is a continuous and piecewise linear function of λ, and

$$\forall \lambda,\ \mathcal{J}(\lambda) = \min_{\{\mathcal{A}\subseteq\{1,\ldots,n\},\ \|\mathcal{A}\|_0 \leqslant \min(m,n)\}} \mathcal{J}_\mathcal{A}(\lambda). \tag{5}$$

Definition 8 *In the following, we will define the values $\lambda = \lambda_i^\star$ ($i = 1,\ldots,I$) as the **critical values**. These values, together with $\lambda_0^\star = 0$ and $\lambda_{I+1}^\star = +\infty$, define the piecewise constant domain $\mathcal{X}_p(\lambda)$:*

$$0 = \lambda_0^\star < \lambda_1^\star < \ldots < \lambda_I^\star < \lambda_{I+1}^\star = +\infty. \tag{6}$$

$\lambda_i^\star$ are also the λ-values at which the derivative of $\mathcal{J}$ is changing: at $\lambda = \lambda_i^\star$, $\lambda \mapsto \mathcal{J}(\lambda)$ is not differentiable, and $\mathcal{J}$ is linear on each interval $[\lambda_i^\star, \lambda_{i+1}^\star]$ (see Fig. 1).

Proof 7 *— The result (5) can be illustrated geometrically, by considering the affine curves $\lambda \mapsto \mathcal{J}_\mathcal{A}(\lambda)$ for all the possible supports $\mathcal{A}$ such that $\|\mathcal{A}\|_0 \leqslant \min(m,n)$ (see Fig. 1). Let us prove that (5) holds.*

When λ is fixed, let $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, and let $\mathcal{A} \triangleq \mathcal{A}(\boldsymbol{x}_p(\lambda))$.

- *According to theorem 5, $\|\boldsymbol{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0 \leqslant \min(m,n)$ and $\boldsymbol{x}_p(\lambda) = \boldsymbol{x}_\mathcal{A}$. Thus, $\mathcal{E}(\boldsymbol{x}_p(\lambda)) = \mathcal{E}_\mathcal{A}$ and*
$$\mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda) = \mathcal{J}_\mathcal{A}(\lambda).$$
- *$\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$ implies that for all $\mathcal{A}' \subseteq \{1,\ldots,n\}$ such that $\|\mathcal{A}'\|_0 \leqslant \min(m,n)$,*
$$\mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda) \leqslant \mathcal{J}_{\mathcal{A}'}(\lambda) = \mathcal{J}(\boldsymbol{x}_{\mathcal{A}'};\lambda).$$

Here, we have shown that (5) holds since $\mathcal{J}(\lambda) = \mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda)$.

— $\lambda \mapsto \mathcal{J}(\lambda)$ is a continuous and piecewise linear function of λ because of (5). Since the number of affine curves $\lambda \mapsto \mathcal{J}_\mathcal{A}(\lambda)$ is finite, $\lambda \mapsto \mathcal{J}(\lambda)$ is described by a finite set of values $\{(\lambda_i^\star, \mathcal{E}_{\mathcal{A}_i}, \|\boldsymbol{x}_{\mathcal{A}_i}\|_0),\ i = 0,\ldots,I\}$, where $\lambda_0^\star = 0 < \lambda_1^\star < \ldots < \lambda_I^\star < \lambda_{I+1}^\star = +\infty$. Each value $\lambda_i^\star$ ($i = 1,\ldots,I$) corresponds to the intersection between a pair of affine curves (see Fig. 1), and the restriction of $\mathcal{J}$ to a given interval $[\lambda_i^\star, \lambda_{i+1}^\star]$ is linear:

$$\forall \lambda \in [\lambda_i^\star, \lambda_{i+1}^\star],\ \mathcal{J}(\lambda) = \mathcal{E}_{\mathcal{A}_i} + \lambda\|\boldsymbol{x}_{\mathcal{A}_i}\|_0. \tag{7}$$

In particular, for $i = 0$, we have

$$\forall \lambda \in [0, \lambda_1],\ \mathcal{J}(\lambda) = \mathcal{E}_{\mathcal{A}_0} + \lambda\|\boldsymbol{x}_{\mathcal{A}_0}\|_0, \tag{8}$$

where $\mathcal{E}_{\mathcal{A}_0} = \min_{\boldsymbol{x}\in\mathbb{R}^n}\mathcal{E}(\boldsymbol{x})$ is the minimal least-square error, and $\|\boldsymbol{x}_{\mathcal{A}_0}\|_0$ is the minimal L0-norm of the minimizers of $\mathcal{E}$ over $\mathbb{R}^n$. For $i = I$, we have necessarily $\boldsymbol{x}_{\mathcal{A}_I} = \mathbf{0}$ and $\mathcal{E}_{\mathcal{A}_I} = \|\boldsymbol{y}\|^2$, thus

$$\forall\lambda \in [\lambda_I^\star, +\infty),\ \mathcal{J}(\lambda) = \|\boldsymbol{y}\|^2. \tag{9}$$

— For a given interval $[\lambda_i^\star, \lambda_{i+1}^\star]$, let us show that when $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$, $\mathcal{X}_p(\lambda)$ is a constant set. For some given λ-value $\in (\lambda_i^\star, \lambda_{i+1}^\star)$, we consider $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$, then necessarily, the following equivalent equations hold:

$$\begin{aligned} \mathcal{J}(\lambda) &= \mathcal{J}(\boldsymbol{x};\lambda) \\ \mathcal{E}_{\mathcal{A}_i} + \lambda\|\boldsymbol{x}_{\mathcal{A}_i}\|_0 &= \mathcal{E}(\boldsymbol{x}) + \lambda\|\boldsymbol{x}\|_0. \end{aligned}$$

Imagine that $\mathcal{E}_{\mathcal{A}_i} \neq \mathcal{E}(\boldsymbol{x})$, then, necessarily, the two functions $\mathcal{J}(\lambda') = \mathcal{E}_{\mathcal{A}_i} + \lambda'\|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ and $\mathcal{J}(\boldsymbol{x};\lambda') = \mathcal{E}(\boldsymbol{x}) + \lambda'\|\boldsymbol{x}\|_0$ do not coincide for $\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star]\backslash\{\lambda\}$. Moreover, $\mathcal{J}(\boldsymbol{x};\lambda')$ is strictly lower than $\mathcal{J}(\lambda')$ either for $\lambda' \in [\lambda_i^\star, \lambda)$ or for $\lambda' \in (\lambda, \lambda_{i+1}^\star]$. This is in contradiction with (7) and the definition of $\mathcal{J}(\lambda')$ in theorem 6.

We have shown that $\mathcal{E}_{\mathcal{A}_i} = \mathcal{E}(\boldsymbol{x})$. Since $\mathcal{J}(\lambda) = \mathcal{J}(\boldsymbol{x};\lambda)$ and $\lambda > 0$, we deduce that $\|\boldsymbol{x}_{\mathcal{A}_i}\|_0 = \|\boldsymbol{x}\|_0$, and that $\forall\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star]$, $\mathcal{J}(\lambda') = \mathcal{J}(\boldsymbol{x};\lambda')$. Finally, if $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$ and $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$, then $\boldsymbol{x} \in \mathcal{X}_p(\lambda')$ for all $\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star]$. $\mathcal{X}_p(\lambda)$ is then a constant set when $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$, and $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^\star) \cap \mathcal{X}_p(\lambda_{i+1}^\star)$.

Lemma 1 *The function $\lambda \mapsto \mathcal{J}(\lambda)$ is increasing and concave.*

Proof 8 *$\mathcal{J}$ is an increasing and concave function as the minimum of a finite set of increasing and concave functions.*

Lemma 2 *$\mathcal{X}_p(0) \cap \mathcal{X}_p \neq \emptyset$, and if $m \geqslant n$, then $\mathcal{X}_p(0) \subset \mathcal{X}_p$.*

Proof 9 *The application of the result of theorem 6: "for all i, if $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^\star)$" with $i = 0$ yields*

$$\forall\lambda \in (0, \lambda_1^\star),\ \mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(0).$$

Thus, we always have $\mathcal{X}_p(0)\cap\mathcal{X}_p \neq \emptyset$. For $m \geqslant n$, $\mathcal{X}_p(0)$ is formed of only one vector, thus $\forall\lambda \in (0, \lambda_1^\star)$, $\mathcal{X}_p(\lambda) = \mathcal{X}_p(0)$, and $\mathcal{X}_p(0) \subseteq \mathcal{X}_p$. Since $\boldsymbol{y} \neq \mathbf{0}$ and $\boldsymbol{A}$ is full rank, the domain (6) is formed of at least two intervals ($I \geqslant 1$), thus $\mathcal{X}_p(0) \subset \mathcal{X}_p$.

Theorem 7 *For a given λ-value which is distinct from $\lambda_0^\star, \lambda_1^\star, \ldots, \lambda_I^\star$, all the elements of $\mathcal{X}_p(\lambda)$ are of same L0-norm, which is equal to the derivative of $\mathcal{J}(\lambda)$, and yield the same least-square cost.*

Proof 10 *Because of theorem 6, for a given value of i, there exists $\mathcal{A}_i \subseteq \{1, \ldots, n\}$ such that*

$$\forall\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star],\ \mathcal{J}(\lambda') = \mathcal{J}_{\mathcal{A}_i}(\lambda'). \tag{10}$$

Now, let us fix the value of $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$ and let $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$. Because of theorem 6, $\mathcal{X}_p(\lambda')$ is constant for $\lambda' \in (\lambda_i^\star, \lambda_{i+1}^\star)$, and $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda')$ for all $\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star]$. (10) implies that

$$\begin{aligned} \forall\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star],\ \mathcal{J}(\boldsymbol{x}_p(\lambda);\lambda') &= \mathcal{J}_{\mathcal{A}_i}(\lambda') \\ \forall\lambda' \in [\lambda_i^\star, \lambda_{i+1}^\star],\ \mathcal{E}(\boldsymbol{x}_p(\lambda)) + \lambda'\|\boldsymbol{x}_p(\lambda)\|_0 &= \mathcal{E}_{\mathcal{A}_i} + \lambda'\|\boldsymbol{x}_{\mathcal{A}_i}\|_0. \end{aligned} \tag{11}$$

Taking the derivative of (11) yields $\|\boldsymbol{x}_p(\lambda)\|_0 = \|\boldsymbol{x}_{\mathcal{A}_i}\|_0 = \mathcal{J}'(\lambda)$, and then, due to (11), $\mathcal{E}(\boldsymbol{x}_p(\lambda)) = \mathcal{E}_{\mathcal{A}_i}$.

Theorem 8 *Let $\boldsymbol{x}_p(\lambda)$ be a sequence such that $\forall\lambda$, $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$. Then, necessarily, $\|\boldsymbol{x}_p(\lambda)\|_0$ is a decreasing function of λ, and $\mathcal{E}(\boldsymbol{x}_p(\lambda))$ is an increasing function of λ.*

Proof 11

- *Recall that for $i \in \{0, \ldots, I\}$, there exists a set $\mathcal{A}_i$ such that if $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$ and $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, then $\|\boldsymbol{x}_p(\lambda)\|_0 = \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ (see theorem 7);*
- *The first result is a direct consequence of theorem 7: $\forall\lambda \notin \{\lambda_0^\star, \ldots, \lambda_I^\star\}$, $\|\boldsymbol{x}_p(\lambda)\|_0 = \mathcal{J}'(\lambda)$, and of lemma 1: $\mathcal{J}$ is a concave function, thus its derivative (when it is defined) is a decreasing function of λ. At this point, we know that $\lambda \mapsto \|\boldsymbol{x}_p(\lambda)\|_0$ is piecewise constant on $\mathbb{R}_+$, and that its restriction to $\mathbb{R}_+\backslash\{\lambda_0^\star, \ldots, \lambda_I^\star\}$ is decreasing: $\forall i \in \{1, \ldots, I\}$, $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \geqslant \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$. The remaining part is to study the behavior of $\|\boldsymbol{x}_p(\lambda)\|_0$ at $\lambda = \lambda_i^\star$, $i = 0, \ldots, I$.*

  For $i \in \{1, \ldots, I\}$, let us show that $\boldsymbol{x}_p(\lambda_i^\star)$ is such that $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \geqslant \|\boldsymbol{x}_p(\lambda_i^\star)\|_0 \geqslant \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$:

– $\lambda \mapsto \mathcal{J}(\boldsymbol{x}_p(\lambda_i^\star);\lambda)$ *and* $\lambda \mapsto \mathcal{J}(\lambda)$ *coincide at* $\lambda = \lambda_i^\star$*;*

– $\mathcal{J}'(\lambda)$ *is equal to* $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0$ *when* $\lambda \in (\lambda_{i-1}^\star, \lambda_i^\star)$*, and to* $\|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ *when* $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$*.*

– *the derivative of* $\lambda \mapsto \mathcal{J}(\boldsymbol{x}_p(\lambda_i^\star);\lambda)$ *is equal to* $\|\boldsymbol{x}_p(\lambda_i^\star)\|_0$*.*

Due to the definition of $\lambda \mapsto \mathcal{J}(\lambda)$ *in theorem 6, the affine function* $\lambda \mapsto \mathcal{J}(\boldsymbol{x}_p(\lambda_i^\star);\lambda)$ *is necessarily greater or equal to* $\lambda \mapsto \mathcal{J}(\lambda)$ *for* $\lambda \in (\lambda_{i-1}^\star, \lambda_i^\star)$ *and for* $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$*. This implies that* $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \geqslant \|\boldsymbol{x}_p(\lambda_i^\star)\|_0 \geqslant \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$*.*

A similar argument can be given to show that $\|\boldsymbol{x}_p(\lambda_0^\star)\|_0 \geqslant \|\boldsymbol{x}_{\mathcal{A}_0}\|_0$*.*

Finally, we have shown that $\lambda \mapsto \|\boldsymbol{x}_p(\lambda)\|_0$ *is decreasing on* $\mathbb{R}_+$*.*

- *Second result: for a given* $i \in \{1,\dots,I\}$*, the continuity of* $\mathcal{J}$ *at* $\lambda = \lambda_i^\star$ *reads* $\mathcal{E}_{\mathcal{A}_{i-1}} + \lambda_i^\star\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 = \mathcal{E}_{\mathcal{A}_i} + \lambda_i^\star\|\boldsymbol{x}_{\mathcal{A}_i}\|_0$*. Because* $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \geqslant \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$*,* $\mathcal{E}_{\mathcal{A}_{i-1}} \leqslant \mathcal{E}_{\mathcal{A}_i}$*.*

  When λ *varies from 0 to* $+\infty$ *and* $\lambda \notin \{\lambda_1^\star,\dots,\lambda_I^\star\}$*,* $\mathcal{E}(\boldsymbol{x}_p(\lambda))$ *takes sequentially the values* $\mathcal{E}_{\mathcal{A}_i}$*,* $i = 0,\dots,I$*. Thus, the restriction of* $\lambda \mapsto \mathcal{E}(\boldsymbol{x}_p(\lambda))$ *to* $\mathbb{R}_+\backslash\{\lambda_1^\star,\dots,\lambda_I^\star\}$ *is increasing. With similar arguments than in the first result, we can show that for* $i \in \{1,\dots,I\}$*,* $\mathcal{E}_{\mathcal{A}_{i-1}} \leqslant \mathcal{E}(\boldsymbol{x}_p(\lambda_i^\star)) \leqslant \mathcal{E}_{\mathcal{A}_i}$*. Finally,* $\lambda \mapsto \mathcal{E}(\boldsymbol{x}_p(\lambda))$ *is increasing on* $\mathbb{R}_+$*.*

3.3 Cardinality of $\mathcal{X}_p(\lambda)$

It is easy to see that:

- For all $i \in \{1,\dots,I\}$, the cardinality of $\mathcal{X}_p(\lambda_i^\star)$ is larger than 2, because at $\lambda = \lambda_i^\star$, at least two distinct affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda\|\boldsymbol{x}_{\mathcal{A}}\|_0$ intersect (see Fig. 2).
- $\mathcal{X}_p(\lambda)$ is reduced to the unique vector $\mathbf{0}$ for the largest λ-values ($\lambda > \lambda_I^\star \Rightarrow \mathcal{X}_p(\lambda) = \{\mathbf{0}\}$).
- For $\lambda = 0$ (the least-square error $\mathcal{E}(\boldsymbol{x})$ is minimized with no penalty), $\mathcal{X}_p(0)$ is either reduced to the unique vector $(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}$ when $m \geqslant n$, or is of infinite cardinality otherwise.

We conclude that at least for $m \geqslant n$, the cardinality of $\mathcal{X}_p(\lambda)$ is not monotonic w.r.t. λ.

3.4 Relationship between the constrained and the penalized solution paths

Generally, the solution paths $\mathcal{X}_c$ and $\mathcal{X}_p$ do not coincide. This is a consequence of the non-convexity of the L0-norm [2]. However, $\mathcal{X}_p \subseteq \mathcal{X}_c$ is always true (a well-known result in the literature of multi-objective optimization?).

In general, the proposition "$\forall k$, $\exists\lambda$, $\mathcal{X}_c(k) \subseteq \mathcal{X}_p(\lambda)$" is false (see Fig. 1).

Theorem 9 *If* $\lambda \neq \{\lambda_0^\star,\dots,\lambda_I^\star\}$*, then there exists* k *such that* $\mathcal{X}_p(\lambda) = \mathcal{X}_c(k)$*.*

Proof 12 *For a given* λ*-value, let* $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$*, let* $\mathcal{A} \triangleq \mathcal{A}(\boldsymbol{x})$ *denote the support of* $\boldsymbol{x}$ *and* $k_{\boldsymbol{x}} \triangleq \|\boldsymbol{x}\|_0 = \|\mathcal{A}\|_0$*. According to theorem 5,* $\|\mathcal{A}\|_0 \leqslant \min(m,n)$ *and* $\boldsymbol{x} = \boldsymbol{x}_{\mathcal{A}}$*.*

— Let us show that $\boldsymbol{x} \in \mathcal{X}_c(k_{\boldsymbol{x}})$*. If* $\boldsymbol{x} \notin \mathcal{X}_c(k_{\boldsymbol{x}})$*, there exists a (minimal) support* $\mathcal{B}$ *such that* $\|\mathcal{B}\|_0 \leqslant k_{\boldsymbol{x}}$ *and* $\mathcal{E}_{\mathcal{B}} < \mathcal{E}(\boldsymbol{x}) = \mathcal{E}_{\mathcal{A}}$*, then* $\mathcal{J}(\boldsymbol{x}_{\mathcal{B}};\lambda) < \mathcal{J}(\boldsymbol{x}_{\mathcal{A}};\lambda)$*. This is in contradiction with* $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$*.*

At this point, we have shown that

$$\forall\lambda,\ \forall\boldsymbol{x} \in \mathcal{X}_p(\lambda),\ \exists k_{\boldsymbol{x}},\ \boldsymbol{x} \in \mathcal{X}_c(k_{\boldsymbol{x}}),$$

or equivalently,

$$\mathcal{X}_p \subseteq \mathcal{X}_c.$$

— The following of the proof requires the assumption $\lambda \neq \{\lambda_0^\star,\dots,\lambda_I^\star\}$*. We have seen that if* $\boldsymbol{x}$ *and* $\boldsymbol{y} \in \mathcal{X}_p(\lambda)$*, then* $\boldsymbol{x} \in \mathcal{X}_c(k_{\boldsymbol{x}})$ *and* $\boldsymbol{y} \in \mathcal{X}_c(k_{\boldsymbol{y}})$*. According to theorem 7, all the elements of* $\mathcal{X}_p(\lambda)$ *are of same L0-norm. Therefore,* $k_{\boldsymbol{y}} = k_{\boldsymbol{x}}$*. At this point, we have shown that*

$$\forall\lambda \neq \{\lambda_0^\star,\dots,\lambda_I^\star\},\ \exists k_\lambda,\ \mathcal{X}_p(\lambda) \subseteq \mathcal{X}_c(k_\lambda).$$

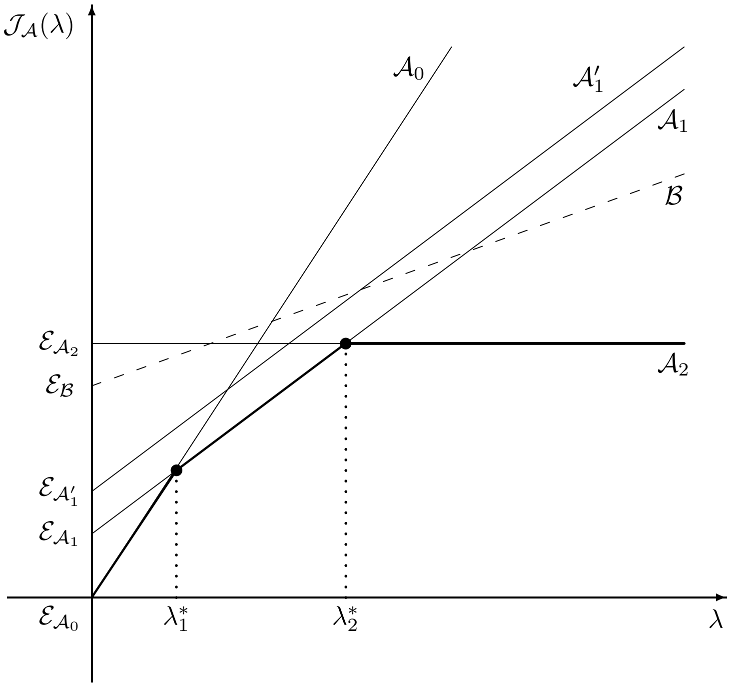

Figure 1: Representation of the affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda\|\boldsymbol{x}_{\mathcal{A}}\|_0$ for all the possible supports $\mathcal{A}$ such that $\|\mathcal{A}\|_0 \leqslant \min(m, n)$. Note that a given affine curve may correspond to several supports $\mathcal{A}$ and $\mathcal{B}$ for which $\forall\lambda$, $\mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{J}_{\mathcal{B}}(\lambda)$. The piecewise linear function $\lambda \mapsto \mathcal{J}(\lambda)$ is defined according to (5) and is represented in bold lines. From this illustration, let us comment on the nonequivalence of both solution paths $\mathcal{X}_c$ and $\mathcal{X}_p$. By following the bold curve representing $\lambda \mapsto \mathcal{J}(\lambda)$, we see that the penalized solution path is described by the active sets $\mathcal{A}_0$, $\mathcal{A}_1$ and $\mathcal{A}_2$ (and the possible other sets yielding the same three curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}_i}(\lambda)$) for which $\|\boldsymbol{x}_{\mathcal{A}}\|_0$ is equal to 3, 2 and 0, respectively. $\mathcal{A}'_1$ is an active set such that $\|\boldsymbol{x}_{\mathcal{A}'_1}\|_0 = 2$ but $\mathcal{E}_{\mathcal{A}'_1} > \mathcal{E}_{\mathcal{A}_1}$. No active set such that $\|\boldsymbol{x}_{\mathcal{A}}\|_0 = 1$ is present in $\mathcal{X}_p$. $\mathcal{B}$ is the active set such that $\|\boldsymbol{x}_{\mathcal{B}}\|_0 = 1$ whose energy $\mathcal{E}_{\mathcal{B}}$ is the lowest among all the active sets such that $\|\boldsymbol{x}_{\mathcal{A}}\|_0 \leqslant 1$, however, $\forall\lambda$, $\mathcal{J}_{\mathcal{B}}(\lambda) > \mathcal{J}(\lambda)$. Thus, $\mathcal{X}_c(1) = \{\boldsymbol{x}_{\mathcal{B}}\} \not\subset \mathcal{X}_p$. On the contrary, for all $\lambda \neq \{\lambda_0^\star, \ldots, \lambda_I^\star\}$, $\mathcal{X}_p(\lambda) = \mathcal{X}_c(k_\lambda)$, with $k_\lambda = \mathcal{J}'(\lambda) = 3$, 2 or 0.

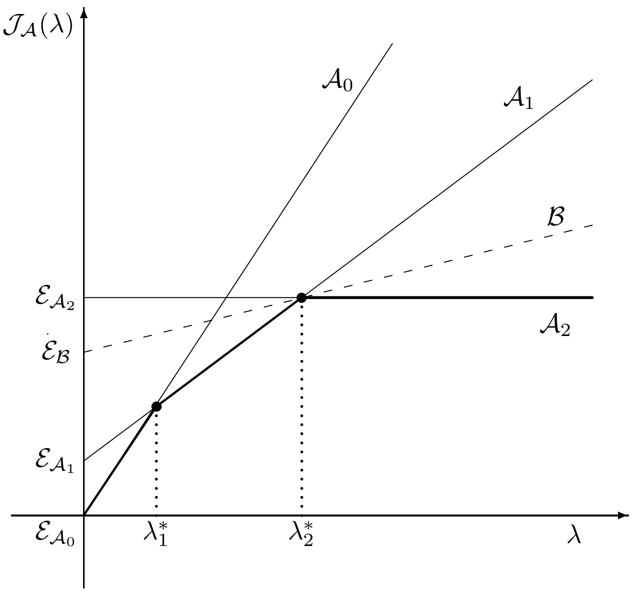

Figure 2: Content of $\mathcal{X}_p(\lambda)$ at a critical λ-value $\lambda = \lambda_i^\star$, $i \geqslant 1$: $\mathcal{X}_p(\lambda_i^\star) \subset \mathcal{X}_c$, and $Card(\mathcal{X}_p(\lambda_i^\star)) \geqslant 2$. On this example, $\mathcal{X}_p(\lambda_2^\star) = \mathcal{X}_c(0) \cup \mathcal{X}_c(1) \cup \mathcal{X}_c(2)$ and $Card(\mathcal{X}_p(\lambda_2^\star)) \geqslant 3$ since $\boldsymbol{x}_{\mathcal{A}_1}$, $\boldsymbol{x}_{\mathcal{A}_2}$ and $\boldsymbol{x}_{\mathcal{B}} \in \mathcal{X}_p(\lambda_2^\star)$.

— Now, let us prove the reverse inclusion. Given λ, there exists at least one $\boldsymbol{x}$ such that $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$, $k_\lambda = \|\boldsymbol{x}\|_0$ and $\boldsymbol{x} \in \mathcal{X}_c(k_\lambda)$. For all $\boldsymbol{y} \in \mathcal{X}_c(k_\lambda)$, we have necessarily $\mathcal{E}(\boldsymbol{y}) = \mathcal{E}(\boldsymbol{x})$ and $\|\boldsymbol{y}\|_0 \leqslant \|\boldsymbol{x}\|_0$, thus $\mathcal{J}(\boldsymbol{y};\lambda) \leqslant \mathcal{J}(\boldsymbol{x};\lambda)$. Since $\boldsymbol{x} \in \mathcal{X}_p(\lambda)$, we deduce that $\mathcal{J}(\boldsymbol{y};\lambda) = \mathcal{J}(\boldsymbol{x};\lambda)$ and that $\boldsymbol{y} \in \mathcal{X}_p(\lambda)$. This completes the proof, since we have shown that

$$\forall \lambda \neq \{\lambda_0^\star, \ldots, \lambda_I^\star\},\ \mathcal{X}_c(k_\lambda) \subseteq \mathcal{X}_p(\lambda).$$

Actually, $k_\lambda = \mathcal{J}'(\lambda)$ according to theorem 7.

3.5 Content of $\mathcal{X}_p(\lambda)$ at critical λ-values

Lemma 3 *If $\lambda_{i-1}^\star < \lambda < \lambda_i^\star < \lambda' < \lambda_{i+1}^\star$, then $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') = \emptyset$.*

Proof 13 *According to theorem 7, all the vectors of $\mathcal{X}_p(\lambda)$ (respectively of $\mathcal{X}_p(\lambda')$) are of same L0-norm, which is the derivative of $\mathcal{J}$ at λ (resp. λ'). Thus, if $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') \neq \emptyset$, the derivative of $\mathcal{J}$ is constant on $(\lambda_{i-1}^\star, \lambda_{i+1}^\star)\backslash\{\lambda_i^\star\}$, which is in contradiction with the definition of $\lambda_i^\star$ (critical point, at which the derivative of $\mathcal{J}$ is changing).*

Theorem 10 *If $\lambda_{i-1}^\star < \lambda < \lambda_i^\star < \lambda' < \lambda_{i+1}^\star$, then $\mathcal{X}_p(\lambda) \cup \mathcal{X}_p(\lambda') \subseteq \mathcal{X}_p(\lambda_i^\star)$, thus $Card(\mathcal{X}_p(\lambda)) + Card(\mathcal{X}_p(\lambda')) \leqslant Card(\mathcal{X}_p(\lambda_i^\star))$ (Card denotes the cardinality). If $\lambda \in (\lambda_{i-1}^\star, \lambda_{i+1}^\star)\backslash\{\lambda_i^\star\}$, then $Card(\mathcal{X}_p(\lambda)) < Card(\mathcal{X}_p(\lambda_i^\star))$.*

See illustration in Fig. 2.

Proof 14
- *First result: according to theorem 6, if $\lambda \in (\lambda_i^\star, \lambda_{i+1}^\star)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^\star) \cap \mathcal{X}_p(\lambda_{i+1}^\star)$. According to lemma 3, if $\lambda_{i-1}^\star < \lambda < \lambda_i^\star < \lambda' < \lambda_{i+1}^\star$, then $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') = \emptyset$. Thus, $\mathcal{X}_p(\lambda) \cup \mathcal{X}_p(\lambda') \subseteq \mathcal{X}_p(\lambda_i^\star)$ and $Card(\mathcal{X}_p(\lambda)) + Card(\mathcal{X}_p(\lambda')) \leqslant Card(\mathcal{X}_p(\lambda_i^\star))$.*
- *Second result: since neither $\mathcal{X}_p(\lambda)$ nor $\mathcal{X}_p(\lambda')$ is empty, their cardinality is larger or equal to 1, then, applying $Card(\mathcal{X}_p(\lambda)) + Card(\mathcal{X}_p(\lambda')) \leqslant Card(\mathcal{X}_p(\lambda_i^\star))$, we deduce that $Card(\mathcal{X}_p(\lambda)) < Card(\mathcal{X}_p(\lambda_i^\star))$ and $Card(\mathcal{X}_p(\lambda')) < Card(\mathcal{X}_p(\lambda_i^\star))$.*

4 SBR and CSBR algorithms

4.1 SBR iterates and output

Let us consider the SBR algorithm for a given λ-value. An SBR iterate takes the form of:

- an active set $\mathcal{A}$ (for simplicity, we omit the dependence w.r.t. λ);
- the corresponding least-square minimizer $\boldsymbol{x}_{\mathcal{A}} = \underset{\{\boldsymbol{x}\in\mathbb{R}^n,\, \mathcal{A}(\boldsymbol{x})\subseteq\mathcal{A}\}}{\arg\min} \mathcal{E}(\boldsymbol{x})$.

$\widehat{\boldsymbol{x}}(\lambda) \triangleq \boldsymbol{x}_{\mathcal{A}}$ is chosen as the estimator of a minimizer (there may be several) of $\mathcal{J}(\boldsymbol{x};\lambda) = \mathcal{E}(\boldsymbol{x}) + \lambda\|\boldsymbol{x}\|_0$ over $\mathbb{R}^n$.

First, recall that for the SBR iterates (and in particular when SBR terminates), $\|\boldsymbol{x}_{\mathcal{A}}\|_0 = \|\mathcal{A}\|_0$. This property can be guaranteed by including in the SBR loops a small procedure which removes from the active set $\mathcal{A}$ all the indices $i \in \mathcal{A}$ such that $\boldsymbol{x}_{\mathcal{A}}(i) = 0$ (however, these removals rarely occur in practice). The following remark follows from this property.

Remark 3 *For a given λ-value, the cost of an SBR iterate $\boldsymbol{x}_{\mathcal{A}}$ is $\mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda\|\mathcal{A}\|_0$. Because the cost of SBR iterates only depend on their support and for convenience, we will omit their dependence w.r.t. $\boldsymbol{x}$.*

Remark 4 *SBR terminates after a finite number of iterations. Moreover, a set $\mathcal{A}$ cannot be explored twice while running SBR.*

Proof 15 *SBR is a descent algorithm and the number of sets $\mathcal{A}$ which are reachable is finite (i.e., the number of subsets of $\{1,\dots,n\}$).*

Remark 5 *When SBR terminates, the estimate $\widehat{\boldsymbol{x}}(\lambda) = \boldsymbol{x}_{\mathcal{A}}$ is generally not included in $\mathcal{X}_p(\lambda)$ because SBR is a sub-optimal algorithm.*

Remark 6 *At the SBR output $\mathcal{A}$, $\mathcal{J}$ is "locally minimum w.r.t. $\mathcal{A}$": any replacement of $\mathcal{A}$ by $\mathcal{A}\bullet i$ (where $\bullet \triangleq \cup$ or $\backslash$) does not yield a decrease of the cost $\mathcal{J}_{\mathcal{A}}(\lambda)$). Formally, this property reads:*

$$\forall i,\ \mathcal{J}_{\mathcal{A}}(\lambda) \leqslant \mathcal{J}_{\mathcal{A}\bullet i}(\lambda), \tag{12}$$

or equivalently,

$$\begin{aligned} \forall i,\ \mathcal{E}_{\mathcal{A}} + \lambda\|\mathcal{A}\|_0 &\leqslant \mathcal{E}_{\mathcal{A}\bullet i} + \lambda\|\boldsymbol{x}_{\mathcal{A}\bullet i}\|_0 \\ \forall i,\ \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\bullet i} &\leqslant \lambda\big(\|\boldsymbol{x}_{\mathcal{A}\bullet i}\|_0 - \|\mathcal{A}\|_0\big). \end{aligned} \tag{13}$$

Here, we do not consider the small removal procedure described above for $\mathcal{A}\bullet i$ (update of $\mathcal{A}\bullet i$ by removing the indices corresponding to the zero valued entries of $\boldsymbol{x}_{\mathcal{A}\bullet i}$), therefore we use $\|\boldsymbol{x}_{\mathcal{A}\bullet i}\|_0$, which may be lower than $\|\mathcal{A}\bullet i\|_0$.

4.2 Iterative computation of λ in the CSBR algorithm

When $\lambda = \lambda_q > 0$ (q-th call to SBR), let $\mathcal{A} = \mathcal{A}_q$ be the support of the output of SBR(λ_q). Then, (13) holds. For simplicity, we will omit, when possible, the dependence of $\mathcal{A}$ w.r.t. q. When λ_q is replaced by another value $\lambda \leqslant \lambda_q$ and $\mathcal{A} = \mathcal{A}_q$ is kept fixed, for which λ-values does (13) remain valid?

When $\bullet = \backslash$, both terms on the left- and right-hand sides of the inequality are strictly negative ($\|\boldsymbol{x}_{\mathcal{A}\backslash i}\|_0 \leqslant \|\mathcal{A}\|_0 - 1$), while when $\bullet = \cup$, both terms are positive since $\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i} \geqslant 0$ and (13) holds for $\lambda = \lambda_q$ (this implies that $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0$ or $\|\mathcal{A}\|_0 + 1$). Therefore, (13) remains valid for $\lambda \neq \lambda_q$ *if and only if*

$$(0 \leqslant) \max_{i\notin\mathcal{A} \text{ and } \|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0+1} (\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i}) \leqslant \lambda \leqslant \min_{i\in\mathcal{A}} \left[\frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\backslash i}}{\|\boldsymbol{x}_{\mathcal{A}\backslash i}\|_0 - \|\mathcal{A}\|_0}\right]. \tag{14}$$

The lower bound of (14) can be simplified to $\max_{i\notin\mathcal{A}}(\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i})$ because if $i \notin \mathcal{A}$ is such that $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0$, then (13) implies that $\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i} = 0$. Thus, including these indices i in the computation of the lower bound of (14) does not change its value, and (14) simplifies to

$$\max_{i\notin\mathcal{A}}(\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i}) \leqslant \lambda \leqslant \min_{i\in\mathcal{A}}\left[\frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\setminus i}}{\|\boldsymbol{x}_{\mathcal{A}\setminus i}\|_0 - \|\mathcal{A}\|_0}\right]. \tag{15}$$

Given λ_q, the next λ-value $\lambda_{q+1} < \lambda_q$ is found by computing the lower bound of (15).

How to choose λ_{q+1}? Setting λ_{q+1} to the lower bound of (15) is not judicious, since for this λ-value, $\mathcal{J}$ is still "locally minimum w.r.t. $\mathcal{A}$" in the sense of (12). One possibility is to set λ_{q+1} to the lower bound of (15) minus some $\varepsilon > 0$, without guarantee that this value is larger than the "next lower bound" of (15). Another possibility is to sort the values of

$$\widetilde{\lambda_i} \triangleq \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\cup i} \geqslant 0 \tag{16}$$

for all indices $i \notin \mathcal{A}$, and then to **set λ_{q+1} to the mean of the two largest values**. This setting ensures that the inequality $\widetilde{\lambda_i} \leqslant \lambda_{q+1}$ does not hold for one value of $\widetilde{\lambda_i}$ only.

- If the number of indices $i \notin \mathcal{A}$ such that $\widetilde{\lambda_i} > 0$ is equal to 1, then we set λ_{q+1} to half of the value of $\widetilde{\lambda_i}$.
- If all indices $i \notin \mathcal{A}$ are such that $\widetilde{\lambda_i} = 0$, then we terminate CSBR.
- If $\mathcal{A}$ is the complete set $\{1, \ldots, n\}$, the lower bound of (15) is undefined, and we terminate CSBR.

Remark 7 *For a given $i \notin \mathcal{A}$ for which $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0 + 1$, $\widetilde{\lambda_i}$ is the λ-value for which both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}\cup i}(\lambda)$ intersect. Similarly, for $i \in \mathcal{A}$, the value*

$$\widetilde{\lambda_i} \triangleq \frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A}\setminus i}}{\|\boldsymbol{x}_{\mathcal{A}\setminus i}\|_0 - \|\mathcal{A}\|_0} \tag{17}$$

is the λ-value for which both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}\setminus i}(\lambda)$ intersect.

Proof 16 *For $i \notin \mathcal{A}$ and for the λ-value $\widetilde{\lambda_i}$, (13) is an equality, then $\mathcal{J}_{\mathcal{A}}(\lambda_i) = \mathcal{J}_{\mathcal{A}\cup i}(\lambda_i)$. Since $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0$ is supposed to be different from $\|\mathcal{A}\|_0$, both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}\cup i}(\lambda)$ are not parallel (their slopes are equal to $\|\mathcal{A}\|_0$ and $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0 + 1$ respectively), and they intersect at $\lambda = \lambda_i$. A similar proof holds in the case where $i \in \mathcal{A}$ and $\cup$ is replaced by $\setminus$.*

Remark 8 *A set $\mathcal{A}$ of cardinality larger than $\min(m, n)$ cannot be explored.*

Proof 17 *— SBR: if a set $\mathcal{A}$ of cardinality larger than $\min(m, n)$ is explored, then SBR has earlier explored at least one set $\mathcal{B}$ of cardinality $\min(m, n)$ (recall that the initial solution is $\mathcal{A} = \emptyset$). Due to the URP assumption, $\mathcal{E}_{\mathcal{B}} = \mathcal{E}_{\mathcal{A}} = \min_{\boldsymbol{x}\in\mathbb{R}^n} \mathcal{E}(\boldsymbol{x})$ is the optimal least-square cost. Therefore, $\|\mathcal{A}\|_0 > \|\mathcal{B}\|_0 \Rightarrow \forall\lambda > 0$, $\mathcal{J}_{\mathcal{A}}(\lambda) > \mathcal{J}_{\mathcal{B}}(\lambda)$. This cannot occur because SBR is a descent algorithm.*

— CSBR. Recursively, for each $\lambda = \lambda_q$, if the initial set $\mathcal{A}_{q-1}$ (input of SBR(λ_q)) is of cardinality lower than $\min(m, n)$, then the output $\mathcal{A}_q$ of SBR(λ_q) is also of cardinality lower than $\min(m, n)$.

4.3 Termination of CSBR

Remark 9 *When CSBR terminates, $\mathcal{E}_{\mathcal{A}} = \mathcal{J}_{\mathcal{A}}(0)$ is locally minimum w.r.t. $\mathcal{A}$, then $\forall i \notin \mathcal{A}$, $\mathcal{E}_{\mathcal{A}\cup i} = \mathcal{E}_{\mathcal{A}}$.*

Remark 10 *CSBR terminates after a finite number of SBR iterations.*

Proof 18
- *According to remark 4, for a given λ-value λ_q, SBR(λ_q) terminates after a finite number of iterations.*
- *According to remark 7, each value of λ_q is such that there exists $\underline{\mu_q}$ and $\overline{\mu_q}$ such that*

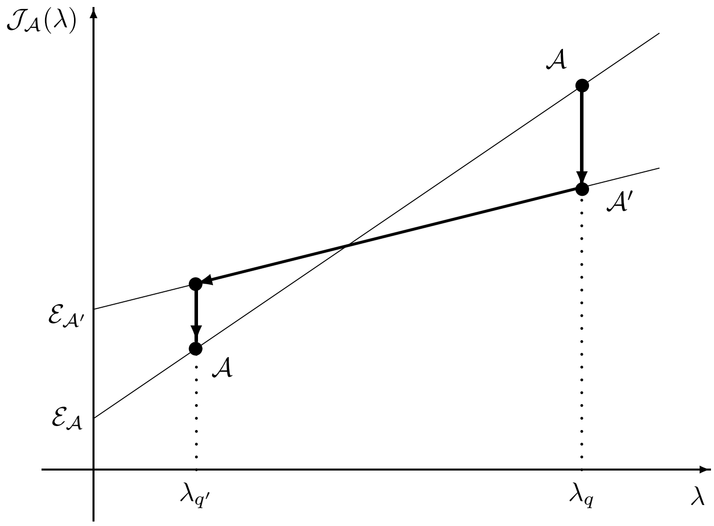

Figure 3: A given set $\mathcal{A}$ may be explored twice during the CSBR procedure, at different λ-values. Here, each vertical line corresponds to one call to SBR ($\mathcal{A}$ and $\mathcal{A}$' are two SBR iterates at λ_q and λ'_q), *i.e.*, to a fixed λ-value while the plain lines are the affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}'}(\lambda)$.

- $0 \leqslant \underline{\mu_q} \leqslant \lambda_q \leqslant \overline{\mu_q}$;
- $\lambda_q = (\underline{\mu_q} + \overline{\mu_q})/2$;
- $\underline{\mu_q}$ *and* $\overline{\mu_q}$ *are critical values for which two affine curves* $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ *and* $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda \cup i)$ *intersect.*

From the recursive construction of the sequence $(\lambda_q, q \geqslant 0)$*, it is clear that* $\forall q$, $\overline{\mu_q} < \lambda_{q-1}$*, thus* $\forall q$, $\overline{\mu_q} < \overline{\mu_{q-1}}$*. Since each value of* $\overline{\mu_q}$ *can be associated to a given intersection between two affine curves* $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ *and* $\lambda \mapsto \mathcal{J}_{\mathcal{B}}(\lambda)$ *and the number of possible subsets* $\mathcal{A}$ *and* $\mathcal{B}$ *of* $\{1, \ldots, n\}$ *whose cardinality is lower than* $\min(m, n)$ *is finite, the number of possible values taken by* $\overline{\mu_q}$ *is also finite. Since the sequence* $(\overline{\mu_q}, q \geqslant 0)$ *satisfies* $\forall q$, $\overline{\mu_q} < \overline{\mu_{q-1}}$*, we conclude that the number of iterations* q *at which SBR(*λ_q*) is run is finite.*

Despite remark 10, we cannot claim that a given set $\mathcal{A}$ is never explored twice during the CSBR procedure. In remark 4, we have seen that a given set $\mathcal{A}$ can never be explored twice while running SBR for a given λ-value. However, $\mathcal{A}$ may be explored several times while running CSBR, *i.e.*, once while running SBR at some λ-value λ_q, and another time while running SBR at another λ-value $\lambda_{q'} \leqslant \lambda_q$ (for $q' > q$). See Fig. 3 for a simple illustration.

Remark 11 *When CSBR terminates, the solution* $\boldsymbol{x}_{\mathcal{A}}$ *is an unconstrained least-square estimate.*

Proof 19 *Let us define the residual* $\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}_{\mathcal{A}}$ *and the unit vectors* $\boldsymbol{e}_i \in \mathbb{R}^n$ *in which all entries are equal to 0 except the* i*-th entry, equal to 1. Then,* $\boldsymbol{A}\boldsymbol{e}_i = \boldsymbol{a}_i$*, where* $\boldsymbol{a}_i$ *stands for the* i*-th column of* $\boldsymbol{A}$*.*

Firstly, we prove that $\forall i \notin \mathcal{A}$, $\boldsymbol{a}_i^T \boldsymbol{r} = 0$*. According to remark 9,* $\mathcal{A}$ *is such that* $\forall i \notin \mathcal{A}$, $\mathcal{E}_{\mathcal{A} \cup i} = \mathcal{E}_{\mathcal{A}}$*. Then, the following inequalities hold:*

$$\begin{aligned}
&\forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R},\ \mathcal{E}(\boldsymbol{x}_{\mathcal{A}} + \varepsilon \boldsymbol{e}_i) - \mathcal{E}(\boldsymbol{x}_{\mathcal{A}}) \geqslant 0 \\
&\forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R},\ \|\boldsymbol{r} - \varepsilon \boldsymbol{a}_i\|^2 - \|\boldsymbol{r}\|^2 \geqslant 0 \\
&\forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R},\ \varepsilon^2 \|\boldsymbol{a}_i\|^2 - 2\varepsilon \boldsymbol{a}_i^T \boldsymbol{r} \geqslant 0 \\
&\forall i \notin \mathcal{A}, \quad \boldsymbol{a}_i^T \boldsymbol{r} = 0.
\end{aligned}$$

Secondly, because $\boldsymbol{x}_{\mathcal{A}}$ is a solution to the constrained problem (2)*:*

$$\begin{array}{ll} \forall i \in \mathcal{A}, & \forall \varepsilon \in \mathbb{R},\ \mathcal{E}(\boldsymbol{x}_{\mathcal{A}} + \varepsilon \boldsymbol{e}_i) - \mathcal{E}(\boldsymbol{x}_{\mathcal{A}}) \geqslant 0 \\ \forall i \in \mathcal{A}, & \boldsymbol{a}_i^T \boldsymbol{r} = 0. \end{array}$$

Finally, we deduce that

$$\begin{array}{rcl} \forall i \in \{1, \dots, n\},\ \boldsymbol{a}_i^T \boldsymbol{r} & = & 0 \\ \boldsymbol{A}^T \boldsymbol{r} & = & \mathbf{0} \\ \boldsymbol{A}^T \boldsymbol{A} \boldsymbol{x}_{\mathcal{A}} - \boldsymbol{A}^T \boldsymbol{y} & = & \mathbf{0} \\ \nabla \mathcal{E}(\boldsymbol{x}_{\mathcal{A}}) & = & \mathbf{0}. \end{array}$$

Since $\mathcal{E}$ is quadratic, we have shown that $\boldsymbol{x}_{\mathcal{A}}$ is an unconstrained least-square estimate.

References

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